ANOMALOUS CROSSOVER BEHAVIOUR FOR DISSIPATIVE TUNNELLING

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We analyzed numerically a metastable system which is coupled to a single bath oscillator with frequency ω_c. If the fequency in the metastable well ω_0 is larger than the bath frequency ω_c we find that the crossover temperature is *increased* with increasing coupling strength. This is in contrast to the usual behaviour that coupling renders the system more classical, thereby lowering the crossover temperature with increasing coupling strength.

1. INTRODUCTION

Initiated by the work of Caldeira and Leggett (CL) (1), there is continuous interest in the influence of environment on tunneling. Whereas CL considered the effect of dissipation at zero temperature for which they found suppression of tunneling, the theory, which is based on the instanton formalism, was extended by Grabert et al. (2) to include finite temperatures T. Their main result was that the tunneling rate is increased at low temperatures according to an exponential T^2 law. Moreover it was shown (3) that the theory is able to bridge between the tunneling dominated escape and classical hopping around the crossover temperature T_c. Quite recently it was demonstrated (4) that the whole range of temperatures is covered in a unfied manner by multidimensional quantum transition state theory.

The crossover temperature T_c may be defined by comparison of the Arrhenius formula for the rate of decay $\sim\exp(-V^{\#}/k_B T)$ for a barrier of height $V^{\#}$ to the WKB expression for transmission through the parabolic barrier of the same height $\sim\exp(-V^{\#}2\pi/\mu)$ with frequency μ. The expressions become comparable at the temperature

$$T_c = \hbar\mu/2\pi k_B. \tag{1}$$

In the dissipative case μ is the normal mode frequency at the barrier top along the unstable reactive mode. This definition of the crossover temperature, however, seems not to be valid for environmental baths which have a cutoff ω_c such that $\omega_c < \omega_0$, where ω_0 is the system frequency in the well.

2. CROSSOVER

In order to study the crossover behaviour we analyzed the CL Hamiltonian with a single bath oscillator, i.e. a cubic potential V(q) with well frequency ω_0 coupled to a harmonic oscillator with frequency ω_c, i.e.

$$H = \frac{p_q^2}{2M} + V(q) + \frac{p_x^2}{2m} + \frac{m}{2}\left\{\omega_c x + \frac{C}{m\omega_c} q\right\}^2 . \tag{2}$$

Resonance energies of this system, that is energies E_n^k and their corresponding decay widths Γ_n^k may then be computed numerically (5) by the method of complex scaling (6) , the pair n,k denotes the excitation level along the system and the bath normal modes, respectively. The complex scaling transformation (CS), crudely speaking, renders the divergent resonance wave function into a bounded one, thus enabling the search for resonance eigenvalues directly on the transformed Hamiltonian in a usual bound state representation. CS is defined by replacing each coordinate y and momentum p_y by $y\exp(i\theta_y)$ and $p_y\exp(-i\theta_y)$ respectively, where the scaling angle θ_y may be complex in general.

Given the complex resonance energies, the thermal decay rate may readily be computed. However the numerical convergence of resonance states with $E_n^0 \geq V^{\#}$ is poor. This limits the evaluation of the thermal rate up to temperatures below crossover since increasingly higher states contribute significantly to the rate with increasing temperature. Nevertheless it is just this effect which provides a different way to study the crossover regime. To this end we consider the relative contributions Γ_n to the rate stemming from the excitation level n along the system mode, including all excitations along the bath mode.

$$\Gamma_n = \sum_{k=0}^{\infty} \Gamma_n^k \exp(-E_n^k/k_B T) \qquad (3)$$

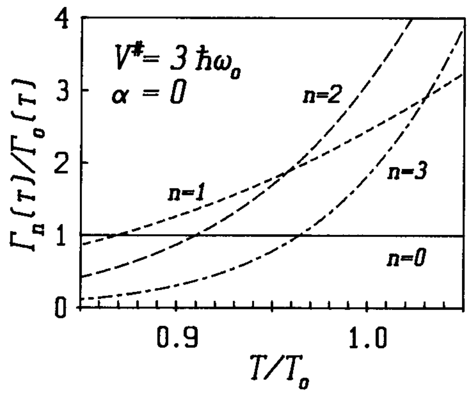

FIGURE 1

Figure 1 displays the reduced quantity Γ_n/Γ_0 for the uncoupled case $\alpha \equiv \pi C^2/(4Mm\omega_0^4)=0$ and the system excitation levels n=0,1,2,3 as a function of tempeature which is normalized to the bare crossover temperature $T_c(\alpha=0)=\hbar\omega_0/2\pi k_B \equiv T_0$. For low temperatures the main contribution to the rate comes from the ground state n=0. With increasing temperature first level n=1 and then level n=2 surmount the ground state contribution. At still higher temperature level n=2 wins over n=1 and contribution of level n=3 increases considerably marking the onset of crossover.

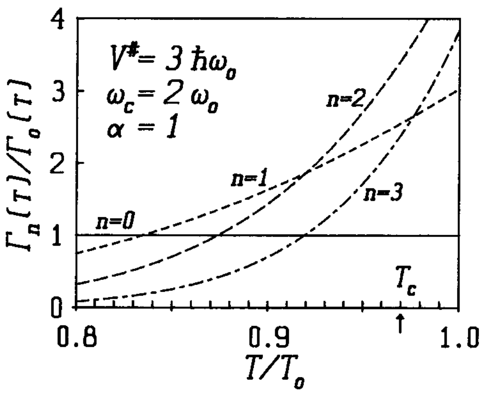

FIGURE 2

Figure 2 shows the same quantities as figure 1 but with a coupling strength $\alpha=1$, and $\omega_c=2\omega_0$, i.e. $\mu/\omega_0 \equiv T_c/T_0=0.969$. The occurences of the events described in figure 1 are now shifted to lower temperatures which means that the crossover for this system starts at lower temperatures in accordance with prediction by eq.(1).

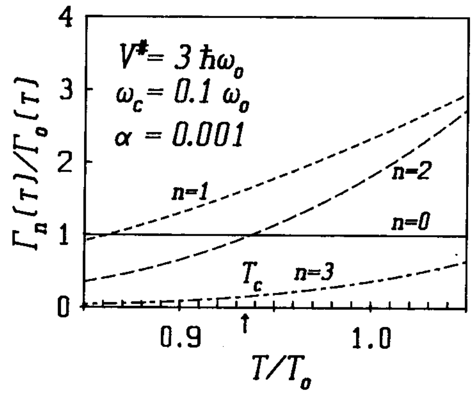

FIGURE 3

Figure 3 also displays Γ_n/Γ_0 but for parameters $\alpha=0.001$ and $\omega_c=0.1\omega_0$, i.e. $\mu/\omega_0=0.935$. Now one observes that the onset of significant contribution to the rate from levels n=1,2,3 is shifted to *higher* temperatures. This clearly indicates that for systems with $\omega_c<\omega_0$ the crossover temperature with coupling T_c is *higher* than the bare crossover tempeature (5), i.e. $T_c>T_0$. This however is in contrast to the bahaviour found for the case $\omega_c>\omega_0$ and the prediction of eq.(1) (note that the reactive normal mode frequency at the barrier is *always* lowered by coupling).

We have demonstrated that for coupling to an oscillator whose frequency ω_c is *lower* than the frequency ω_0 in the metastable well the crossover behaviour is anomalous. At present it is however not clear whether this remains true for a cutoff bath with a continuous frequency distribution.

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